

Cluster Heat Bath Algorithm in Monte Carlo Simulations of Ising Models

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Abstract

We have proposed a cluster heat bath method in Monte Carlo simulations of Ising models in which one of the possible spin configurations of a cluster is selected in accordance with its Boltzmann weight. We have argued that the method improves slow relaxation in complex systems and demonstrated it in an axial next-nearest-neighbor Ising(ANNNI) model in two-dimensions.

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Recently various algorithms have been proposed to reduce the CPU time of computer in the Monte Carlo(MC) simulation [1]. Cluster-flip algorithms [2,3] were proposed using ideas from percolation theory [4]. Although the methods were very efficient to simulate large systems near criticality, these were not successfully applied to complex systems which contain frustrated interactions such as spin-glasses. On the other hand, to study the ordered state of complex systems, extended ensemble methods were developed [5–8]. In these methods, however, the conventional single-spin-flip algorithm is used to guarantee the ergodicity. Quite recently, a new update method was proposed in which the spin configuration of a chain of Ising spins is updated in accordance with the Boltzmann weight [9]. The method is very effective for quasi-one-dimensional models and enables us to make realistic simulations [10] of quasi-one-dimensional Ising magnets such as CsCoBr_3 [11] and CsCoCl_3 [12]. However, it was not so useful for ordinary two- and three-dimensional models, especially for complex systems.

In this Letter, we propose a general configuration-update algorithm which is applicable to various Ising models with short-range interactions and very effective for improving slow relaxation in complex systems. We consider to find the probable spin configuration of a cluster of N spins. This can be readily done when N is small, but becomes difficult when N is increased. However, if the cluster is decomposed into layers of spins and interlayer couplings exist only between the spins on adjacent layers, we can update the spin configuration of the layers step by step with the aid of a transfer matrix technique. Thus, we can treat a larger cluster, e.g., a cluster of $N \sim M \times L$ spins in a cubic lattice with the nearest neighbor couplings, where L is the linear size of the lattice and M is the number of the spins of the layer. We can prove that the spin configuration realized in this method is in accordance with the Boltzmann weight. So we call the algorithm a cluster heat bath (CHB) method. We argue that the CHB method improves slow relaxation in complex systems and demonstrate it in an axial next-nearest-neighbor Ising (ANNNI) model [13] in two-dimensions.

We start with an Ising model described by the Hamiltonian

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j, \quad (1)$$

where $\sigma_i (= \pm 1)$ are Ising spins and J_{ij} are coupling constants. Now we pick out a cluster of spins and consider its probable spin configuration under the condition that the other spins are fixed. It is noted that the cluster defined here is *an ensemble of connected spins in a fixed part of the system*, not one of connected spins with the same sign. We suppose that the cluster is composed of L layers and interactions exist only between neighboring layers. Hereafter we call the cluster as A_L . The Hamiltonian of A_L is, then, described as

$$\mathcal{H}_{A_L} = - \sum_{l=1}^{L-1} H_{l,l+1} - \sum_{l=1}^L B_l, \quad (2)$$

with

$$H_{l,l+1} = \sum_i \sum_j J_{ij}^{(l,l+1)} \sigma_i^{(l)} \sigma_j^{(l+1)}, \quad (3)$$

$$B_l = \sum_{ij} J_{ij}^{(l)} \sigma_i^{(l)} \sigma_j^{(l)} + \sum_i h_i^{(l)} \sigma_i^{(l)}, \quad (4)$$

where $J_{ij}^{(l)}$ and $J_{ij}^{(l,l+1)}$ are exchange interactions between i th and j th spins on the same layer (l) and those between different layers (l) and ($l+1$), respectively. The effective field $h_i^{(l)}$ of i th spin on the layer (l) is given as a sum of the external field and the exchange field which comes from the spins surrounding A_L :

$$h_i^{(l)} = \sum_j J_{ij} \sigma_j + mH, \quad (5)$$

where m and H are the magnetic moment and the external field, respectively.

Now we consider the probable spin configuration $\{\sigma_i^{(L)}\}$ of the layer (L). We define the following weight function $F_l(\{\sigma_i^{(l)}\})$:

$$F_l(\{\sigma_i^{(l)}\}) = \sum_{\{\sigma_i^{(1)}=\pm 1\}} \cdots \sum_{\{\sigma_i^{(l-1)}=\pm 1\}} \exp(\beta \sum_{k=1}^{l-1} H_{k,k+1} + \beta \sum_{k=1}^l B_k), \quad (6)$$

where $\beta = 1/k_B T$ with k_B and T being the Boltzmann's constant and temperature, respectively. This function can be readily obtained from the recursion formula

$$F_l(\{\sigma_i^{(l)}\}) = \sum_{\{\sigma_i^{(l-1)}=\pm 1\}} F_{l-1}(\{\sigma_i^{(l-1)}\}) \exp(\beta H_{l-1,l} + \beta B_l) \quad l \geq 2 \quad (7)$$

with the initial function $F_1(\{\sigma_i^{(1)}\}) = \exp(\beta B_1)$. The probability $P_L(\{\sigma_i^{(L)}\})$ of the spin configuration $\{\sigma_i^{(L)}\}$ of the layer (L) is given as

$$P_L(\{\sigma_i^{(L)}\}) = \frac{F_L(\{\sigma_i^{(L)}\})}{Z_L}, \quad (8)$$

where $Z_L (= \sum_{\{\sigma_i^{(L)} = \pm 1\}} F_L(\{\sigma_i^{(L)}\}))$ is the partition function of A_L . Thus, we can determine the spin configuration $\{\sigma_i^{(L)}\}$ of the layer (L) using a uniform random number.

The next step is to determine the spin configuration $\{\sigma_i^{(L-1)}\}$ of the layer $(L-1)$ under the condition that the spin configuration of the layer (L) is given as $\{\sigma_i^{(L)}\}$. This is equivalent to determine the spin configuration $\{\sigma_i^{(L-1)}\}$ of the cluster A_{L-1} which is obtained by removing the layer (L) from A_L . The spins on this layer (L) of A_L now contribute to the effective fields on the layer $(L-1)$ of A_{L-1} . Thus, the effective field $\tilde{h}_i^{(L-1)}$ of the i th spin on the layer $(L-1)$ of A_{L-1} is given as

$$\tilde{h}_i^{(L-1)} = h_i^{(L-1)} + \sum_j J_{ij}^{(L-1,L)} \sigma_j^{(L)}. \quad (9)$$

Then, the function $F_{L-1}(\{\sigma_i^{(L-1)}\})$ of A_L becomes

$$\begin{aligned} \tilde{F}_{L-1}(\{\sigma_i^{(L-1)}\}) &= \sum_{\{\sigma_i^{(L-2)} = \pm 1\}} F_{L-2}(\{\sigma_i^{(L-2)}\}) \exp(\beta H_{L-2,L-1} + \beta B_{L-1} + \beta H_{L-1,L}) \\ &= F_{L-1}(\{\sigma_i^{(L-1)}\}) \exp(\beta H_{L-1,L}) \end{aligned} \quad (10)$$

for A_{L-1} . The probability $P_{L-1}(\{\sigma_i^{(L-1)}\})$ of the spin configuration $\{\sigma_i^{(L-1)}\}$ of the layer $(L-1)$ is given as

$$P_{L-1}(\{\sigma_i^{(L-1)}\}) = \frac{\tilde{F}_{L-1}(\{\sigma_i^{(L-1)}\})}{\tilde{Z}_{L-1}} \quad (11)$$

with

$$\begin{aligned} \tilde{Z}_{L-1} &= \sum_{\{\sigma_i^{(L-1)} = \pm 1\}} \tilde{F}_{L-1}(\{\sigma_i^{(L-1)}\}) \\ &= F_L(\{\sigma_i^{(L)}\}) \exp(-\beta B_L). \end{aligned} \quad (12)$$

Thus, we can also determine the spin configuration $\{\sigma_i^{(L-1)}\}$ of the layer $(L-1)$. Repeating this procedure from the layer $(L-1)$ to the layer (1) , the spin configuration of the cluster A_L can be updated.

We can readily show that the spin configuration of A_L realized in this procedure is in accordance with the Boltzmann weight. The probability of this spin configuration $P_{A_L}(\{\sigma_i^{(1)}\}, \{\sigma_i^{(2)}\}, \dots, \{\sigma_i^{(L)}\})$ is given as the product of the individual probabilities $P_l(\{\sigma_i^{(l)}\})$, i.e.,

$$\begin{aligned} P_{A_L}(\{\sigma_i^{(1)}\}, \{\sigma_i^{(2)}\}, \dots, \{\sigma_i^{(L)}\}) &= \prod_{l=1}^L P_l(\{\sigma_i^{(l)}\}) \\ &= \prod_{l=1}^{(L-1)} \frac{\tilde{F}_l(\{\sigma_i^{(l)}\})}{\tilde{Z}_l} \times \frac{F_L(\{\sigma_i^{(L)}\})}{Z_L} \\ &= \frac{1}{Z_L} \exp(-\beta \mathcal{H}_{A_L}). \end{aligned} \tag{13}$$

This is nothing but the Boltzmann weight. Hence we call this algorithm a cluster heat bath (CHB) method. When all the spins are updated one time, we call it one MC sweep just like in the conventional MC method.

The CHB method can be applied to clusters with any shape. It is not necessary that the interactions of the model are of the nearest neighbor. Only restriction is that we can decompose the cluster into layers as described in the form of eq. (2). It is most effective to choose the cluster as ladders with its width of M in two-dimensions and columns with its intersection of $M_x \times M_y$ in three-dimensions, because we can use the transfer matrix technique [14]. The CHB method may improve relaxation in various systems. The updated spin configuration of the cluster depends on its environment but not on its original spin configuration. Thus, the spin structure may always fluctuate in the scale of the cluster size and, of course, a cluster-flip effect is automatically taken into account [15]. Moreover, if we choose the cluster appropriate to the model, we may perform most effective MC simulation. Here, we demonstrate it in a simulation of the ANNNI model [13] in two-dimensions.

The ANNNI model is an array of Ising chains with ferromagnetic interaction J_1 between spins in adjacent chains and competing antiferromagnetic interaction J_2 between spins in next-nearest-neighbor chains, augmented by ferromagnetic nearest-neighbor interaction J_0 in the chains. It is well known that, for $\kappa \equiv -J_2/J_1 > \frac{1}{2}$, the ground state of the model is the $(2, \bar{2})$ antiphase described by an alternate arrangement of two up-spin chains and two

down-spin chains, i.e., $\cdots ++ -- ++ \cdots$. It is believed that a floating incommensurate(IC) phase appears between the $(2, \bar{2})$ antiphase and the paramagnetic phase. However, it turned out to be much CPU time consuming to establish the phase boundaries reliably [13]. The difficulty in the MC simulation of the ANNNI model is that the spin structure depends on initial spin configurations. This is because the spin structure of the IC phase near transition to the $(2, \bar{2})$ antiphase consists of regions of the $(2, \bar{2})$ antiphase separated by $+++$ or $---$ walls [16]. Therefore, it is necessary to insert 4 walls simultaneously to the $(2, \bar{2})$ antiphase to get the IC phase starting from the $(2, \bar{2})$ antiphase. That is, we must rearrange at least $16N_x$ spins to get the IC phase, where N_x is the number of the spins of the chain, which is not easy to be realized by using the conventional single-spin-flip MC method [17]. This difficulty is not largely relieved even when we choose an open boundary condition, because open boundaries lead to a pinning effect [18], i.e., the end two chains tend to take either $++$ or $--$ configuration. In this case, we must rearrange at least $8N_x$ spins at the ends. So the ANNNI model is one of the most difficult models in the computer simulation [13]. However, if we use the CHB method with clusters of $M \times N_x$ spins with $M \geq 16$ (or $M \geq 8$ at the ends), we may easily add or remove the walls.

To examine our speculation, we performed the CHB simulation of the model with $J_0 = J_1$ and $\kappa = 0.6$ on the lattice of $N_x \times N_y = 64 \times 128$ spins with open boundary conditions. We treated clusters of 8×64 spins [19]. At each temperature, we started with two different initial spin configurations, i.e., a paramagnetic spin configuration and the $(2, \bar{2})$ antiphase spin configuration, and calculated quantities of interest. Here we present results of the square of the chain magnetization M_2 which plays the role of the order parameter of this model [20,21]:

$$M_2 = \frac{1}{N_y} \sum_j^{N_y} \left(\frac{1}{N_x} \sum_i^{N_x} \sigma_{ij} \right)^2. \quad (14)$$

As temperature is decreased below $T = 1.0J_1$, the relaxation becomes very slow. We present, in Figs. 1(a) and 1(b), typical results of the MC sweep dependence of M_2 at $T = 0.9J_1$ in the conventional MC and CHB methods, respectively. Figure 1(a) shows most clearly the

difficulty of the computer simulation of the ANNNI model as mentioned above. However, we could get its equilibrium value within a reasonable number of MC sweeps using the CHB method as seen in Fig. 1(b). We calculated the average values $\langle M_2 \rangle$ at different temperatures using both the methods. Results are presented in Figs. 2(a) and 2(b) for the conventional MC method and the CHB method, respectively. At all temperatures, in the CHB method, we could get the same values starting with the two initial spin configurations in contrast with the conventional MC method [22]. Thus, we conclude that the CHB method, in fact, relieve the difficulty of the computer simulation of the ANNNI model.

We have proposed a new update algorithm of the spin configuration and demonstrated its efficiency in the ANNNI model in two-dimensions. We should note again that the algorithm is a natural generalization of the conventional heat bath algorithm and applicable to various systems with short-range interactions. Since a large fluctuation of the spin configuration may occur for every MC sweep, the CHB method is particularly useful for studying equilibrium properties of complex systems such as spin-glasses [23]. We also note that we may perform much more effective MC simulation by combining the CHB method with extended ensemble methods such as the exchange MC method [8].

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numbers of connected spins which may flip simultaneously are limited. However, if in each of the clusters there exist many spin configurations which have almost the same energy, one of them is selected in accordance with its Boltzmann weight.

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FIGURES

FIG. 1. The MC sweep dependences of the order parameter M_2 at $T = 0.9J_1$ starting with two initial spin configurations of a paramagnetic phase (PARA) and the $(2, \bar{2})$ antiphase (AP) by (a) the conventional MC method and (b) the CHB method.

FIG. 2. The temperature dependences of the average value of the order parameter $\langle M_2 \rangle$ starting with two initial spin configurations of a paramagnetic phase (PARA) and the $(2, \bar{2})$ antiphase (AP) by (a) the conventional MC method and (b) the CHB method. In the conventional MC method, the averages were taken over $2 \times 10^4 - 4 \times 10^4$ and $1 \times 10^5 - 1.5 \times 10^5$ MC sweeps for $T \geq 1.0J_1$ and $T \leq 0.9J_1$, respectively. On the other hand, in the CHB method, those were taken over much smaller numbers of MC sweeps, i.e., $5 \times 10^2 - 10 \times 10^2$ and $1 \times 10^4 - 1.5 \times 10^4$ MC sweeps for $T \geq 1.0J_1$ and $T \leq 0.9J_1$, respectively.

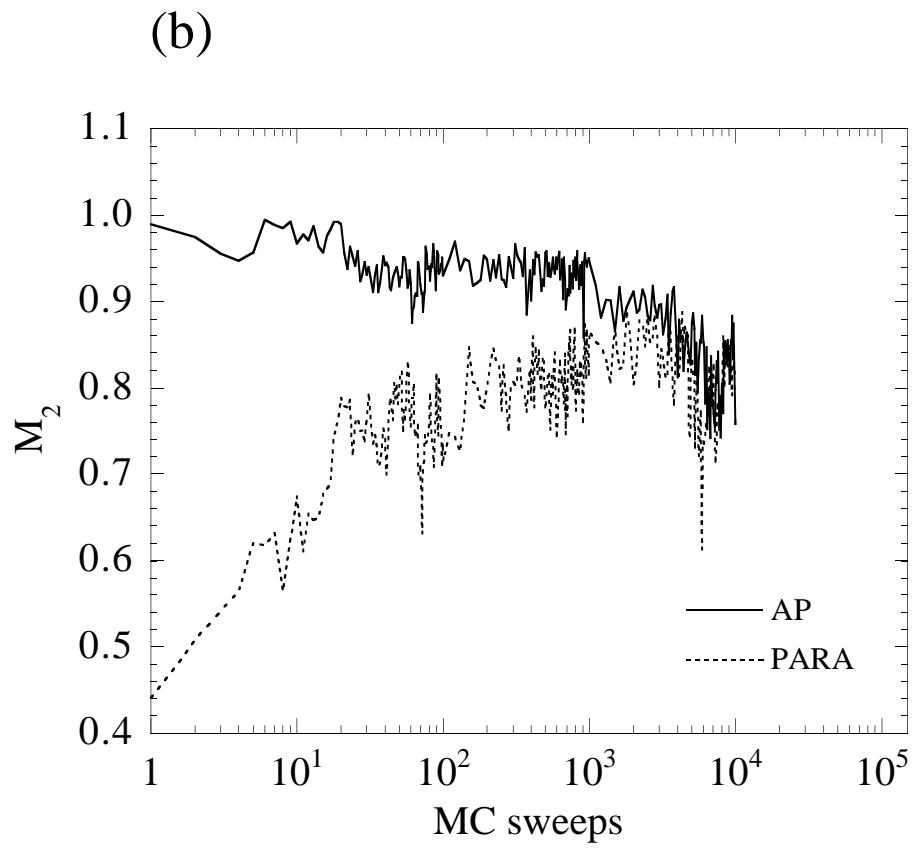
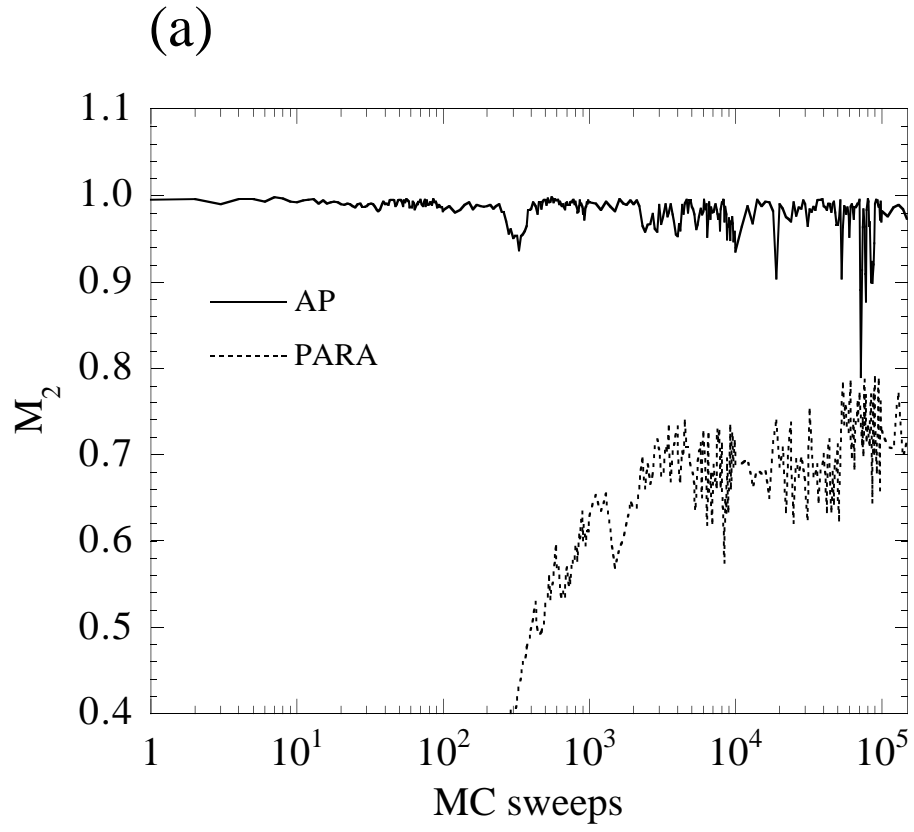


FIG.1. F. Matsubara et al.

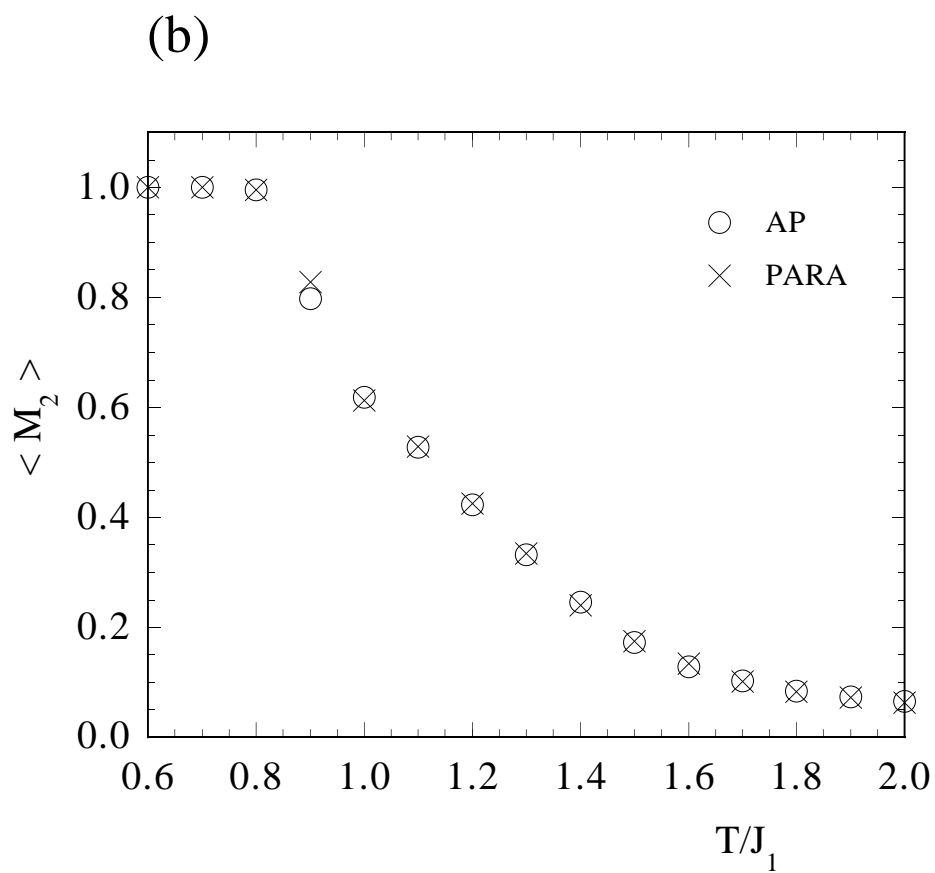
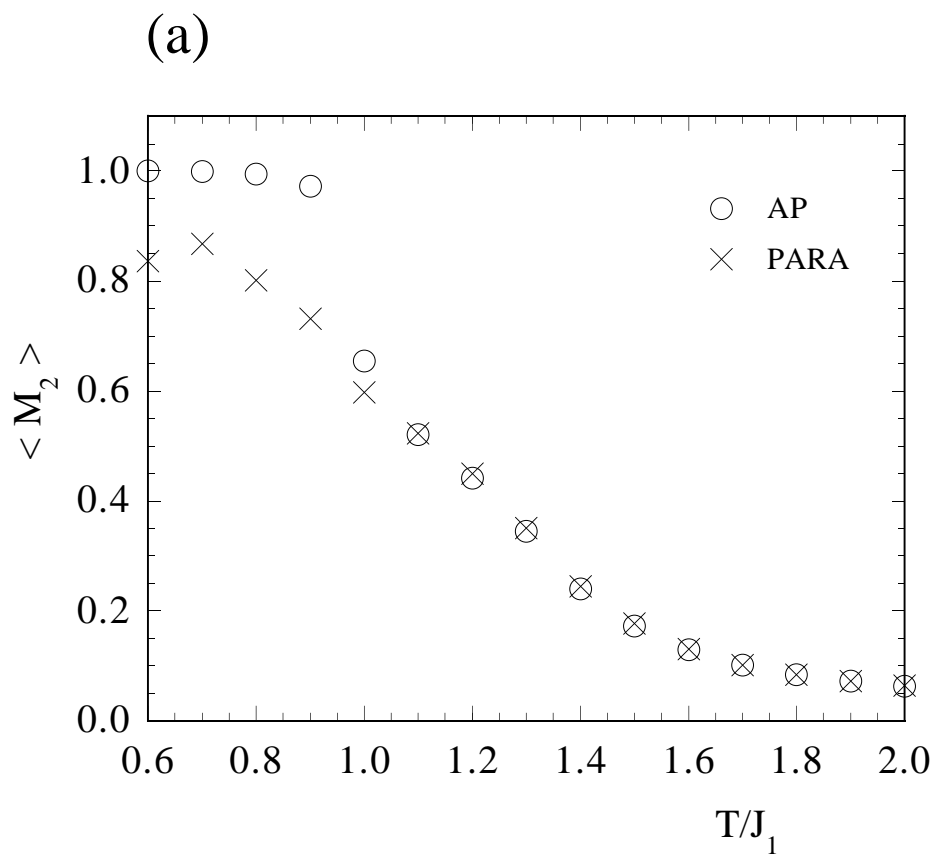


FIG.2. F. Matsubara et al.